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SECURITY CLASSIFICATION OF THIS PAGE

DTIC ELECTE SEP 27 1989 S B D

REPORT DOCUMENTATION PAGE

DTIC FILE COPY

(2)

AD-A212 284

1a. REPORT SECURITY CLASSIFICATION	Unclassified
1b. RESTRICTIVE MARKINGS	
2a. SECURITY CLASSIFICATION AUTHORITY	
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
3. DISTRIBUTION/AVAILABILITY OF REPORT	Approved for public release; distribution unlimited.
5. MONITORING ORGANIZATION REPORT NUMBER(S)	AFOSR-TR- 89-1252
6a. NAME OF PERFORMING ORGANIZATION	University of Michigan
6b. OFFICE SYMBOL (If applicable)	
7a. NAME OF MONITORING ORGANIZATION	AFOSR/NM
6c. ADDRESS (City, State, and ZIP Code)	Ann Arbor, MI, 48109-1027
7b. ADDRESS (City, State, and ZIP Code)	AFOSR/NM Bldg 410 Bolling AFB DC 20332-6448
8a. NAME OF FUNDING/SPONSORING ORGANIZATION	AFOSR
8b. OFFICE SYMBOL (If applicable)	NM
9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER	AFOSR 86-0047
8c. ADDRESS (City, State, and ZIP Code)	AFOSR/NM Bldg 410 Bolling AFB DC 20332-6448

10. SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO.
61102F	2304	A	

11. TITLE (Include Security Classification)

Stochastic Process Models in Device Physics

12. PERSONAL AUTHOR(S)

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13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Final	FROM 06/86 TO 08/89	20 Aug 1989	seven

16. SUPPLEMENTARY NOTATION

17. COSATI CODES

FIELD	GROUP	SUB-GROUP

18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

The aim of this project was to undertake a statistical study of Monte-Carlo methods in device physics using tools from the modern theory ot probability and stochastic processes. The Monte Carlo approach has been used to obtain numerical estimates of parameters by simulating the physical process on a computer rather than attempting to solve the integro-differential equations which arise. Thus this method estimates averages and can be applied to any quantity expressible as such but may require an enormous number of simulations before statistically reliable results are obtained, especially if the quantity of interest is subject to very low probability of occurrence. A probabilistic study was undertaken of the behaviour of individual electrons, complementing the Monte-Carlo approach. The methodology required the formulation of some novel stochastic processes and suggested new types of conditions for ergodicity of Markov processes.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS	unclassified

22a. NAME OF RESPONSIBLE INDIVIDUAL	22b. TELEPHONE (Include Area Code)	22c. OFFICE SYMBOL
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DD FORM 1473, 84 MAR

83 APR edition may be used until exhausted.
All other editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE

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89 9 27 024

AFOSR-TR- 89-1252

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FINAL TECHNICAL REPORT

Stochastic Process Models in Device Physics

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20 August 1989

Final Technical Report for Period 1 June 1986 - 31 May 1988
(extended to 7 Aug. 1989)

Prepared for
UNITED STATES AIR FORCE
Air Force Office of Scientific Research
Code PKZ
Bolling Air Force Base
Washington, D.C. 20332-6448

Grant AFOSR-86-0047

Summary.

The aim of this project was to undertake a statistical study of Monte-Carlo methods in semi-conductor device physics using tools from the modern theory of probability and stochastic processes. The Monte-Carlo approach has been used to obtain numerical estimates of parameters by simulating the physical process on a computer rather than attempting to solve the integro-differential equations which arise. Thus this method estimates averages and can be applied to any quantity expressible as such but may require an enormous number of simulations before statistically reliable results are obtained, especially if the quantity if interest is subject to very low probability of occurrence. A probabilistic study of the behaviour of individual electrons was undertaken, complementing the Monte-Carlo approach. The methodology required the formulation of some novel stochastic processes and suggested new types of conditions for ergodicity of Markov processes.

Research Objectives.

The objective of this project was to undertake a statistical study of Monte-Carlo methods in semi-conductor device physics using tools from the modern theory of probability and stochastic processes. The principle behind a Monte-Carlo transport calculation consists of the simulation on a computer of the motion of an electron as an alternating sequence of free flights (drift) in an external field followed by a collision (scattering) with a phonon or impurity. Between collisions the electron obeys, in the semi-classical approximation, Newton's second law $h\ dk/dt = e\ F$ where e is the electron charge, h Planck's constant, k the wave number, and F the external field. The times between collisions and the final states after collisions are random quantities whose probability distributions are determined by the electric field strength and the transition functions of the scattering events. These pairs of mechanisms, deterministic drift and random scattering, are repeated and a histogram is constructed counting the proportion of time the electron occupies each state. Thus the Monte-Carlo method estimates averages and can be applied to any quantity expressible as an average. It is, in principle, capable of giving accurate results but may require an enormous number of simulations before statistically reliable results are obtained, especially if the quantity if interest involves states having low probability of occurrence.

The stochastic structure of these simulations is quite attractive from a statistical viewpoint, describing what are known as random evolutions and embracing a diversity of topics from stochastic processes. The scattering mechanism, for instance, is known as a self-exciting point process in the probability literature. It was hoped that a probabilistic study of the behaviour of individual electrons would complement the Monte-Carlo approach and provide insight which could not otherwise be obtained. Conversely the physical problem suggested a class of random processes whose probabilistic structure was quite attractive and whose analysis would enrich the subject of stochastic processes.

At the start of this work the P.I. intended to develop close ties with the Electron Physics Laboratory at the University of Michigan in order to acquire first hand details of the substantive issues and to maintain a fruitful collaboration , in particular with Dr Peter Blakey. However Dr Blakey left shortly after work began and consequently the research acquired a more mathematical flavor than originally anticipated.

The main goals of this research were:
1. to formulate the Monte-Carlo approach rigorously as stochastic processes;
2. to prove limit theorems relating to steady state behaviour;
3. to interpret the limit theorems qualitatively as functions of electric field strength and scattering mechanisms which could then be interpreted as identifiable physical properties of semi-conductor material;
4. to determine whether the speed of convergence in the limit theorems could be improved by biasing and if so how feasible it would be to implement computer automated iasing in the Monte-Carlo runs.

Status of the Research

A detailed analysis has been made of a model motivated by the momentum randomizing acoustic phonon scattering in the (100) valley of Gallium Arsenide. This has been extended to processes having an upper and a lower valley with intervalley scattering although these results are less complete.

When an electron in the (100) valley of GaAs undergoes acoustic scattering the energy surface of the final state is spherical and the momentum is uniformly distributed on this surface, unlike, for instance, the non-uniform scattering of polar optical scattering in the (000) valley or intervalley scattering. The mathematical details of this model are as follows. There is a stochastic process k(t) representing the momentum of a particle. The momentum increases linearly with acceleration a between scattering events. These events occur at random times $\{T_n\}$ determined by a self exciting point process according to the infinitesimal rule

$$P[\text{scattering event in time interval } (t,t+Dt) \mid k(s),\ 0\le s\le t\ ] = \lambda(k(t))\ Dt + o(Dt).$$

The process k(t) is Markovian and its behaviour is completely determined by the function $\lambda(k)$, depending on which k(t) may exhibit transient, null recurrent, or ergodic behaviour. While physical considerations demand that k(t) be ergodic, nonetheless all three types of behaviour or possible mathematically. For example if λ grows slowly then few scattering events occur when k is large and the motion is almost deterministic to infinity, hence transient.

To illustrate the nature of the results obtained, the general cases of which are technical and are being prepared for publication, let $\lambda(k)$ = constant = μ^{-1} . Let U_n denote k just after the n^{th} scattering event and V_n k just prior to the n^{th} scattering event

Theorem 1. $U_n \Rightarrow U.$

Theorem 2. $V_n \Rightarrow V.$

Theorem 3. $V = U + aT;$
$U = VZ$

where equality and limits are to be taken in the distributional sense. In the first equation of Theorem 3 U and T are independent on the right side and T is exponential with mean m while in the second equation V and Z are independent and Z is uniform on (-1,1). The methodology involves establishing bounds of the form

$$P[\sup(n \geq N) \; |P \; Z_i| > e \;] \leq \frac{c}{b(1+b)^{N-1}}.$$

Next let $S(t) = \int_0^t k(s)\, ds.$

Theorem 4. $\lim \frac{S(t)}{t} = a\mu$ a.s.

Theorem 5. $\lim \frac{S(t)-a\mu t}{(t/\mu)^{1/2}} = N\ (0,\ s^2)$.

Theorem 4, as ergodic theorem, has a natural interpretation as Ohm's law, since the left side represents the current, a is proportional to the electric field, and m is a function of the medium.

When $\lambda(k) = |k|$ analogously results hold. Thus

$$\lim \frac{S(t)}{t} = Ka^{1/2} \quad \text{a.s. for some constant K.}$$

This displays non-ohmic behaviour. In general

$$\lim \frac{S(t)}{t} = g(a)$$

for some function g which can be described as the solution of a second order ODE.

Necessary and sufficient conditions for ergodicity seem difficult to obtain. The usual approach would be to verify a condition due to Doeblin but this condition is hard to verify and it may not hold. A promising alternative is based on the observation that the transition densities $p(x,y)$ of many of the above models share the following property:

there is a real $c > 0$ such that if $A = \{y : y \leq c\}$ then
$p(x,A) \geq 1/2$ uniformly in x.

Intuitively this should cause the process to return ergodically to each state. The general implications of such a condition are currently under investigation.

Multiple scattering mechanisms have also been formulated by enlarging the state space to a vector stochastic process $(k(t), i(t))$ where i is an index identifying the valley. Scattering events may be one of two types involving either:

(a) change in $k(t)$, no change in $i(t)$;

(b) no change in $k(t)$, change in $i(t)$ (intervalley scattering).

The marginal process $k(t)$ is no longer Markov.

The results described above are currently being prepared for publication.